

1,3-Dimethyl-4-ethylbenzene
874-41-9 | DTXSID0061246

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 5.52e-05 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.76e-01

Confidence level: 6.42e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Terpinolene</div> <div>Measured: 6.97e-05</div> <div>Predicted: 6.64e-05</div>	<div>Image not found</div> <div>Limonene</div> <div>Measured: 7.77e-05</div> <div>Predicted: 5.10e-05</div>	<div>Image not found</div> <div>D-Limonene</div> <div>Measured: 7.77e-05</div> <div>Predicted: 5.10e-05</div>
<div>Image not found</div> <div>gamma-Terpinene</div> <div>Measured: 6.37e-05</div> <div>Predicted: 4.78e-05</div>	<div>Image not found</div> <div>5-Ethylidene-2-norbornene</div> <div>Measured: 7.40e-05</div> <div>Predicted: 2.32e-04</div>	<div>Image not found</div> <div>alpha-Pinene</div> <div>Measured: 1.83e-05</div> <div>Predicted: 3.40e-05</div>